

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.49e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.61e-01

Confidence level: 3.47e-01

Nearest Neighbors from the Training Set

Image not found

Cyclodecane

Measured: 2.92e-06

Predicted: 4.64e-01

Image not found

Acenaphthene

Measured: 5.17e-04

Predicted: 1.84e-03

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2,3,5,6-Tetrachloronitrobenzene

Measured: 1.10e-06

Predicted: 1.20e-03

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Thiophene, 2-bromo-

Measured: 1.95e-05

Predicted: 11.9